

'Non-constrained least squares fit

'Five variables

[Variables]

y=col(7) 'unknown

a=col(2) 'alpha helix

b=col(3) 'antiparallel beta

b2=col(4) 'parallel beta

t=col(5) ' turn

r=col(6) 'remainder

[Parameters]

A = 0.25 ' fraction alpha

B = 0.25 ' fraction antiparallel beta

B2 = 0 ' fraction parallel beta

T = 0.25 ' fraction trun

R = 0.25 ' fraction remainder

C=0

[Equation]

f=A*a+B*b+B2*b2+ T*t+R*r +C

fit f to y

[Constraints]

A>0

B>0

B2>0

T>0

R>0

[Options]

tolerance=0.000100

stepsize=100

iterations=100